2-Propenoic acid, 2-(2-hydroxyethoxy)ethyl ester $13533-05-6\mid \mathsf{DTXSID}5050397$

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.72	51.8	0.74	50.3	0.73	52.7	

Model Results

Predicted value: -37.3 °C

Global applicability domain: Inside

Local applicability domain index: 5.22e-01

Confidence level: 5.81e-01

Nearest Neighbors from the Training Set

Image not found

2-(2-Ethoxyethoxy)ethanol

Measured: -76.0 Predicted: -52.5

Image not found

Dodecanoic acid, 2-(2-hydroxyethoxy)ethyl ester

Measured: 17.5 Predicted: 5.44

Image not found

2-[2-(2-

Methoxyethoxy)ethoxy]ethanol

Measured: -44.0 Predicted: -40.0

Image not found

2-[2-(2-

Ethoxyethoxy)ethoxy]ethanol

Measured: -18.7 Predicted: -32.0

Image not found

Methyl 2-hydroxypropanoate

Measured: -66.0 Predicted: -52.7